Canonically invariant formulation of the semiclassical trace formula in terms of the phase space path integral

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1 Derivation of the semiclassical trace formula

The semiclassical trace formula developed by Gutzwiller is one of the most important tools to study spectra of non-integrable systems. However, the original derivation of this formula is very complicated and the canonical invariance of the formula (especially the Maslov index) is unclear.

In this paper, we examine the semiclassical trace formula using phase space path integral to clarify its canonical structure. We mainly study geometrical structure of the Maslov index [1, 2]. We also explain how to treat continuous symmetries and bifurcations in our formalism.

We start with the phase space path integral of the partition function:

\[ Z(T) = \int \mathcal{D}p \mathcal{D}q \exp \left[ \frac{i}{\hbar} \oint (pdq - H dt) \right]. \]  

(1)

The density of states is obtained as the Fourier-Laplace transformation of the partition function:

\[ \rho(E) = -\frac{1}{\pi} \text{Im}g(E + i\epsilon), \]  

(2)

\[ g(E) = \text{Tr} \frac{1}{E - \hat{H}}, \]  

(3)

\[ = \frac{1}{i\hbar} \int_{0}^{\infty} dt e^{\frac{iET}{\hbar}} Z(T). \]  

(4)

We obtain the semiclassical trace formula by applying the stationary phase approximation to the path integral.

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The stationary phase condition reads
\[
\delta \int (pdq - H dt) = 0, \tag{5}
\]
which leads to the Hamiltonian equation of motion. Since the periodic boundary condition of the path integral (1) has the effect of closing the paths, the solutions of (5) are periodic orbits.

Thus the partition function is approximated by a sum over the periodic orbits:
\[
Z(T) = \sum_{p,a} K \exp \left[ \frac{i}{\hbar} R \right]. \tag{6}
\]
Here, \( R = \int pdq - H dt \) is the classical action of the periodic orbit, and \( K \) is the contribution of the quadratic fluctuation around the orbit:
\[
K = \int Dx \exp [i\delta^2 R[x(t)]], \tag{7}
\]
\[
x(t) = \frac{1}{\sqrt{\hbar}}(\delta q, \delta q). \tag{8}
\]
The Maslov index appears as the phase factor of this quadratic path integral.

2 Geometrical properties of the Maslov index

The quadratic path integral can be written as
\[
K = \int Dx \exp \left[ \frac{i}{2} x^T J \mathcal{D} x \right], \tag{9}
\]
where
\[
\mathcal{D} = J \left( \frac{d}{dt} + A(t) \right) \tag{10}
\]
and
\[
A(t) = J H''(p_{cl}(t), q_{cl}(t)). \tag{11}
\]
Here, \( J \) is the matrix to define the symplectic product, and \( H'' \) is the Hessian on the classical trajectory. This is a kind of gauge theory. The set of displacement vectors \( \{ x(t) \} \) is considered to be a vector bundle over \( S^1 \), and the flow around the orbit define a connection (Fig. 1), which is represented by the gauge field \( A(t) \). A gauge transformation in this theory is a canonical transformation of the displacement vector \( x \).

Since (9) is a Fresnel integral,
\[
K = \frac{e^{-\frac{i}{2} \mu_T}}{|\det \mathcal{D}|}. \tag{12}
\]
\( \mu_T \) is the Maslov index in the time representation, whose formal definition is
\[
\mu_T = \frac{\mu_- - \mu_+}{2}, \tag{13}
\]
The set of displacement vectors is regarded as a fibre bundle, and Hamiltonian symplectic flow defines the connection. The structure group of this space is $Sp(2n, R)$

where $\mu_+ (\mu_-)$ is the number of positive (negative) eigenvalues of $\mathcal{H}$. The Maslov index $\mu$ in the Gutzwiller’s trace formula is related to $\mu_T$ by

$$\mu = \mu_T + \frac{1}{2} \text{sgn} \left( \frac{dE}{dT} \right).$$

Actually $\mu$ does not depend on $dE/dT$ because the second term in the RHS of (14) cancels $dE/dT$-dependence of $\mu_T$.

In fact, both $\mu_+$ and $\mu_-$ in (13) are infinite. Therefore we have to discretize the differential operator $\mathcal{H}$ and take the continuum limit to obtain well-defined $\mu_T$. Another way to calculate $\mu_T$ is to change the gauge field $A(t)$ continuously from a reference point, say, $A = 0$. Then we can see the change of the Maslov index from the spectral flow of $\mathcal{H}$.

In this model, we can locally remove the gauge field $A(t)$ by some gauge transformation. Therefore the connection is characterized by the monodromy matrix $M(t)$, which represents holonomy along the classical path, if we are allow to use all gauge transformations. However, the Maslov index changes if we use topologically non-trivial gauge transformations. This is probably the simplest example of the global anomaly, which has been known in quantum field theories [4, 5].

Since the fundamental group of the symplectic group is $Z$, topology of a gauge transformation is characterized by an integer, which represents the winding number. Therefore the Maslov index is determined by the monodromy matrix (more precisely, its conjugacy class) and the winding number. It was shown in [1, 2] that the Maslov index of the $n$-th repetition of a primitive periodic orbit is

$$\mu_n = \sum_{j=1}^{p} \left( 1 + 2 \left[ \frac{n\alpha_j}{2\pi} \right] \right) + qn + \frac{1}{2} \sum_{l=1}^{r} \text{sgn} \gamma_l + 2kn.$$  \hspace{1cm} (15)

Here, $p$, $q$ and $r$ are the number of elliptic, inverse hyperbolic and parabolic blocks in the monodromy matrix, respectively. $k$ is the winding number of the primitive orbit,
\( \alpha_j \) the stability angle of the \( j \)-th elliptic block, and \( \gamma_l \) the non-diagonal part of the \( l \)-th parabolic block. Note that \( \mu_n \neq n\mu_1 \) in general [3].

### 3 Continuous symmetries and bifurcations

When we consider a system with continuous symmetries, periodic orbits are not isolated, and the normal trace formula diverges. Creagh and Littlejohn[6, 7] have derived generalized trace formulae for systems with continuous symmetries by explicitly performing the trace integral over a manifold formed by the continuous family of the orbits. However, their derivation is not easy, because the integrand is not constant over the manifold.

In our formalism based on (1), in contrast, the integrand is just a constant on the manifold of the degenerate periodic orbits. Therefore derivation of the generalized trace formulae are almost trivial. This example shows the elegance of our formalism.

When a periodic orbit bifurcates, similar divergence happens in the normal trace formula, and we have to use the uniform approximation to treat such problems. If we start with the path integral (1), we have to take into account not only quadratic fluctuations around the orbit, but also higher order terms with respect to a soft mode. This procedure is essentially the same as that in caustic problems [9]. The only difference is the boundary condition of the path integral. Therefore our method shows the conceptual similarity between caustic and bifurcation very clearly. Change of the Maslov index at a bifurcation point can also be understood very intuitively in our formalism.

### 参考文献


